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=> s selenocysteine and (crystal structure or three dimenssional structure) and x-ray
L1          15 SELENOCYSTEINE AND (CRYSTAL STRUCTURE OR THREE DIMENSSIONAL
               STRUCTURE) AND X-RAY

=> d ibib abs 1-15

L1   ANSWER 1 OF 15  CAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2002:977958  CAPLUS
DOCUMENT NUMBER:          138:54541
TITLE:                    Mutated bacterial adhesin proteins for inducing high
                          potency inhibitory antibodies against urinary tract
                          infection
INVENTOR(S):              Langermann, Solomon R.; Hultgren, Scott J.; Hung,
                          Chia-Suei; Bouckaert, Julie
PATENT ASSIGNEE(S):       Medimmune, Inc., USA
SOURCE:                   PCT Int. Appl., 1194 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.         KIND  DATE          APPLICATION NO.   DATE
     ---------------    ----  --------      ---------------   --------
     WO 2002102974      A2    20021227      WO 2001-US47994   20011210
     WO 2002102974      A3    20030522
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
             UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2003199071      A1    20031023      US 2001-15085     20011210
PRIORITY APPLN. INFO.:                     US 2000-254353P   P 20001208
                                           US 2001-301878P   P 20010629
AB   The present invention provides bacterial immunogenic agents for
     administration to humans and non-human animals to stimulate an immune
     response, It particularly relates to the vaccination of mammalian species,
     esp. human patients, with variants of the Escherichia coli FimCH protein
     that elicit antibodies that have better functional inhibitory activity
     than antibodies raised against wild type protein.  In particular, such
     variants include mutations that promote a more open confirmation of the
     FimH protein, particularly in regions involved in mannose binding, to
     expose regions previously poorly exposed and mutations that abolish a
     significantly reduce mannose binding.  In another aspect, the invention
     provides antibodies against such proteins and protein complexes that may
     be used in passive immunization to protect or treat pathogenic bacterial
     infections.  The present invention also provides machine readable media
     embedded with the three-dimensional at. structure coordinates of FimCH
     bound to mannose, and subsets thereof, and methods of using the
     crystal structure to provide candidate amino acid
     residues for mutation.  In addn., the invention provides methods for
     identifying FimC or FimH binding compds. and for computational design of
     the binding compds.

L1   ANSWER 2 OF 15  CAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2002:787882  CAPLUS
DOCUMENT NUMBER:          138:51586
TITLE:                    Structure of the Cathelicidin Motif of Protegrin-3
                          Precursor. Structural Insights into the Activation
                          Mechanism of an Antimicrobial Protein
AUTHOR(S):                Sanchez, Jean-Frederic; Hoh, Francois; Strub,
                          Marie-Paule; Aumelas, Andre; Dumas, Christian
CORPORATE SOURCE:         Centre de Biochimie Structurale, Universite
                          Montpellier I, UMR 554 INSERM, UMR CNRS 5048,
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Montpellier, 34060, Fr.
SOURCE: Structure (Cambridge, MA, United States) (2002), 10(10), 1363-1370
CODEN: STRUE6; ISSN: 0969-2126
PUBLISHER: Cell Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Cathelicidins are a family of antimicrobial proteins isolated from leukocytes and epithelia cells that contribute to the innate host defense mechanisms in mammalians. Located in the C-terminal part of the holoprotein, the cathelicidin-derived antimicrobial peptide is liberated by a specific protease cleavage. Here, we report the **x-ray** structure of the cathelicidin motif of protegrin-3 solved by MAD phasing using the **selenocysteine**-labeled protein. Its overall structure represents a fold homologous to the cystatin family and adopts two native states, a monomer, and a domain-swapped dimer. This **crystal structure** is the first example of a structural characterization of the highly conserved cathelicidin motif and thus provides insights into the possible mechanism of activation of the antimicrobial protegrin peptide.
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:704578 CAPLUS
DOCUMENT NUMBER: 137:212639
TITLE: Cell-free synthesis of heavy atom-containing proteins for **x-ray** crystallography structural analysis
INVENTOR(S): Nunokawa, Emi; Kikawa, Takanori; Yabuki, Takashi; Yokoyama, Shigeyuki
PATENT ASSIGNEE(S): Institute of Physical and Chemical Research, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002262867	A2	20020917	JP 2001-65799	20010308
US 2002168705	A1	20021114	US 2001-989974	20011120

PRIORITY APPLN. INFO.: JP 2001-65799 A 20010308
AB A method for large-scale cell-free synthesis of heavy atom-contg. proteins suitable for **x-ray** crystallog. structural anal. using dialysis, is disclosed. Cell ext. of E. coli, hyperthermophilic archaeon, or yeast, is used. It also includes ATP regeneration system, macromol. adsorbent, and reducing agent. Creatine kinase and creatine phosphate are used for ATP regeneration. Amino acids contg. mercury, platinum, iodine, iron, or selenium, such as **selenocysteine** or selenomethionine, are to be incorporated. Synthesis of selenomethionine-contg. Ras protein by cell-free synthesis system, crystn. by hanging-drop vapor-diffusion method, and structural anal. by multiwavelength anomalous diffraction (MAD), are described. The three dimensional structure model produced was identical to those of unlabeled proteins produced in vivo and in cell-free system.

L1 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:487169 CAPLUS
DOCUMENT NUMBER: 137:212817
TITLE: Structure of external aldimine of Escherichia coli CsdB, an IscS/NifS homolog: implications for its specificity toward **selenocysteine**
AUTHOR(S): Mihara, Hisaaki; Fujii, Tomomi; Kato, Shin-Ichiro; Kurihara, Tatsuo; Hata, Yasuo; Esaki, Nobuyoshi
CORPORATE SOURCE: Institute for Chemical Research, Kyoto University, Kyoto, 611-0011, Japan
SOURCE: Journal of Biochemistry (Tokyo, Japan) (2002), 131(5), 679-685
CODEN: JOBIAO; ISSN: 0021-924X

PUBLISHER: Japanese Biochemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Escherichia coli CsdB is a pyridoxal 5'-phosphate (PLP)-dependent enzyme that catalyzes both cysteine desulfuration and **selenocysteine** deselenation. The enzyme has a high specific activity for L-**selenocysteine** relative to L-cysteine. On the other hand, its paralog, IscS, exhibits higher activity for L-cysteine, which acts as a sulfur donor during the biosynthesis of the iron-sulfur cluster and 4-thiouridine. The structure of CsdB complexed with L-propargylglycine was detd. by **X-ray** crystallog. at 2.8 .ANG. resoln.
The overall polypeptide fold of the complex is similar to that of the uncomplexed enzyme, indicating that no significant structural change occurs upon formation of the complex. In the complex, propargylglycine forms a Schiff base with PLP, providing the features of the external aldimine formed in the active site. The Cys364 residue, which is essential for the activity of CsdB toward L-cysteine but not toward L-**selenocysteine**, is clearly visible on a loop of the extended lobe (Thr362-Arg375) in all enzyme forms studied, in contrast to the corresponding disordered loop (Ser321-Arg332) of the Thermotoga maritima NifS-like protein, which is closely related to IscS. The extended lobe of CsdB has an 11-residue deletion compared with that of the NifS-like protein. These facts suggest that the restricted flexibility of the Cys364-anchoring extended lobe in CsdB may be responsible for the ability of the enzyme to discriminate between selenium and sulfur.
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:368500 CAPLUS
DOCUMENT NUMBER: 136:365761
TITLE: Crystals and three-dimensional structures of bacterial LuxS proteins and their use for design of antibiotic inhibitors
INVENTOR(S): Lewis, Hal A.
PATENT ASSIGNEE(S): Structural Genomix, Inc., USA
SOURCE: PCT Int. Appl., 473 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002038595	A2	20020516	WO 2001-US30684	20011001
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003036091	A1	20030220	US 2000-729838	20001204
AU 2002036434	A5	20020521	AU 2002-36434	20011001

PRIORITY APPLN. INFO.:
US 2000-237933P P 20001003
US 2000-729838 A 20001204
WO 2001-US30684 W 20011001

AB The present invention provides cryst. LuxS, machine-readable media embedded with the three-dimensional at. structure coordinates of LuxS, and subsets thereof, and methods of using them. LuxS protein is involved in the prodn. of autoinducer-2, an intercellular signaling mol. employed in the quorum sensing pathway of various bacteria. Thus, cryst. forms are prepd. for LuxS from Helicobacter pylori, Haemophilus influenzae, and Deinococcus radiodurans, and high-resoln. **x-ray** diffraction structures and at. structure coordinates are obtained. This information is useful for solving the crystal and soln. structures of related and unrelated LuxS proteins, and for screening for, identifying and/or designing compds. that bind and/or modulate a biol. activity of

LuxS. The at. structural information may also be used to design novel mutant forms of LuxS polypeptides.

L1 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:754439 CAPLUS
DOCUMENT NUMBER: 136:81865
TITLE: Modeling the Active Sites in Metalloenzymes 5. The Heterolytic Bond Cleavage of H2 in the [NiFe] Hydrogenase of Desulfovibrio gigas by a Nucleophilic Addition Mechanism
AUTHOR(S): Niu, Shuqiang; Hall, Michael B.
CORPORATE SOURCE: HPCC Group Environmental Molecular Science Laboratory, Battelle Pacific Northwest National Laboratory, Richland, WA, 99352, USA
SOURCE: Inorganic Chemistry (2001), 40(24), 6201-6203
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The H2 activation catalyzed by an Fe(II)-Ni(III) model of the [NiFe] hydrogenase of Desulfovibrio gigas has been investigated by d. functional theory (DFT/B3LYP) calcns. on the neutral and anionic active site complexes, [(CO)(CN)2Fe(.mu.-SH)2Ni(SH)(SH2)]0 and [(CO)(CN)2Fe(.mu.-SH)2Ni(SH)2]-. The results suggest that the reaction proceeds by a nucleophilic addn. mechanism that cleaves the H-H bond heterolytically. The terminal cysteine residue Cys530 in the [NiFe] hydrogenase active site of the D. gigas enzyme plays a crucial role in the catalytic process by accepting the proton. The active site is constructed to provide access by this cysteine residue, and this role explains the change in activity obsd. when this cysteine is replaced by a **selenocysteine**. Furthermore, the optimized geometry of the transition state in the model bears a striking resemblance to the geometry of the active site as detd. by **X-ray** crystallog.
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:634472 CAPLUS
DOCUMENT NUMBER: 135:300447
TITLE: Three-dimensional structure of a mammalian thioredoxin reductase: implications for mechanism and evolution of a **selenocysteine**-dependent enzyme
AUTHOR(S): Sandalova, Tatyana; Zhong, Liangwei; Lindqvist, Yiva; Holmgren, Arne; Schneider, Gunter
CORPORATE SOURCE: Division of Molecular Structural Biology, Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Stockholm, S-171 77, Swed.
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2001), 98(17), 9533-9538
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Thioredoxin (Trx) reductases (TrxRs) from mammalian cells contain an essential **selenocysteine** (Sec) residue in the conserved C-terminal sequence, Gly-Cys-Sec-Gly, forming a selenenyl sulfide in the oxidized enzyme. Redn. by NADPH generates a selenolthiol, which is the active site in the redn. of Trx. Here, the 3-dimensional structure of the Sec498Cys mutant of rat TrxR in complex with NADP was detd. to 3.0 .ANG. resoln. by **x-ray** crystallog. The overall structure was found to be similar to that of glutathione reductase (GR), including conserved amino acid residues binding the cofactors, FAD and NADPH. Surprisingly, all residues directly interacting with the substrate, glutathione disulfide (GSSG) in GR were conserved despite the failure of GSSR to act as a substrate for TrxR. The 16-residue C-terminal tail, which is unique to mammalian TrxR, was found to fold in such a way that it could approach the active site disulfide of the other subunit in the dimer. A model of the complex of TrxR with Trx suggests that electron transfer from NADPH to the disulfide of the substrate is possible without large conformational changes. The C-terminal extension typical of mammalian TrxRs has 2 functions: (1) it extends the electron transport

chain from the catalytic disulfide to the enzyme surface, where it can react with Trx, and (2) it prevents the enzyme from acting as a GR by blocking the redox-active disulfide. These results suggest that mammalian TrxR evolved from the GR scaffold rather than from its prokaryotic counterpart. This evolutionary switch renders cell growth dependent on Se.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:487143 CAPLUS
DOCUMENT NUMBER: 135:149129
TITLE: **Crystal structure** of a NifS homologue CsdB from Escherichia coli
AUTHOR(S): Fujii, Tomomi; Hata, Yasuo
CORPORATE SOURCE: Kyoto Univ., Japan
SOURCE: ICR Annual Report (2001), Volume Date 2000, 7, 48-49
CODEN: IAREFM; ISSN: 1342-0321
PUBLISHER: Kyoto University, Institute for Chemical Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Escherichia coli CsdB is a dimeric NifS-homolog belonging to the fold-type I family of PLP-dependent enzymes, and catalyzes the decompn. of L-**selenocysteine** into selenium and L-alanine with specificity higher than that for a substrate of cysteine. The structure of the enzyme has been detd. at 2.8 .ANG. resoln. by an **x-ray** crystallog. method. The subunit of CsdB comprises a large domain, a small domain, and an N-terminal segment. A remarkable structural feature of CsdB is that an .alpha.-helix in the lobe extending from the small domain to the large domain in one subunit of the dimer interacts with a .beta.-hairpin loop protruding from the large domain of the other subunit. Cys364, which is essential for the activity toward cysteine but not toward **selenocysteine**, is clearly seen on the loop of the extended lobe (Thr362-Arg375) although the corresponding loop (Ser321-Arg332) is disordered in the Thermotoga maritima NifS-like protein, which is closely related to the cysteine-specific NifS and whose **crystal structure** has recently been detd. as the second example.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:889773 CAPLUS
DOCUMENT NUMBER: 134:172682
TITLE: Allium chemistry: synthesis, natural occurrence, biological activity, and chemistry of Se-alk(en)ylselenocysteines and their .gamma.-glutamyl derivatives and oxidation products
AUTHOR(S): Block, Eric; Birringer, Marc; Jiang, Weiqin; Nakahodo, Tsukasa; Thompson, Henry J.; Toscano, Paul J.; Uzar, Horst; Zhang, Xing; Zhu, Zongjian
CORPORATE SOURCE: Department of Chemistry, State University of New York-Albany, Albany, NY, 12222, USA
SOURCE: Journal of Agricultural and Food Chemistry (2001), 49(1), 458-470
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:172682

AB Syntheses are reported for .gamma.-glutamyl Se-methylselenocysteine (8a), selenolanthionine (16), Se-1-propenylselenocysteine (6d), Se-2-methyl-2-propenyl-L-**selenocysteine** (6e), and Se-2-propynyl-L-**selenocysteine** (6f). Oxidn. of 8a and Se-methylselenocysteine (6a) gives methaneseleninic acid (24), characterized by **X-ray** crystallog., and di-Me diselenide (25). Oxidn. of Se-2-propenyl-L-**selenocysteine** (6c) gives allyl alc. and 3-seleninoalanine (22). Compd. 22 is also formed on oxidn. of 16 and selenocystine (4). Oxidn. of 6d gives 2-[(E,Z)-1-propenylseleno]propanal (36). These oxidns. occur by way of selenoxides, detected by chromatog. and spectroscopic methods. The natural occurrence of many of the Se-alk(en)ylselenocysteines and their

.gamma.-glutamyl derivs. and oxidn. products is discussed. Three homologues of the potent cancer chemoprevention agents 6a and 6c, namely 6d-f, were evaluated for effects on cell growth, induction of apoptosis, and DNA-damaging activity using two murine mammary epithelial cell lines. Although each compd. displays a unique profile of activity, none of these compds. (6d-f) is likely to exceed the chemopreventive efficacy of **selenocysteine** Se-conjugates 6a and 6c.

REFERENCE COUNT: 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:50772 CAPLUS
DOCUMENT NUMBER: 132:218803
TITLE: Structure of a NifS Homologue: **X-ray** Structure Analysis of CsdB, an Escherichia coli Counterpart of Mammalian **Selenocysteine** Lyase
AUTHOR(S): Fujii, Tomomi; Maeda, Masaki; Mihara, Hisaaki; Kurihara, Tatsuo; Esaki, Nobuyoshi; Hata, Yasuo
CORPORATE SOURCE: Institute for Chemical Research, Kyoto University, Uji Kyoto, 611-0011, Japan
SOURCE: Biochemistry (2000), 39(6), 1263-1273
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Escherichia coli CsdB, a NifS homolog with a high specificity for L-**selenocysteine**, is a pyridoxal 5'-phosphate (PLP)-dependent dimeric enzyme that belongs to aminotransferases class V in fold-type I of PLP enzymes and catalyzes the decompn. of L-**selenocysteine** into selenium and L-alanine. The **crystal structure** of the enzyme has been detd. by the **X-ray** crystallog. method of multiple isomorphous replacement and refined to an R-factor of 18.7% at 2.8 .ANG. resoln. The subunit structure consists of three parts: a large domain of an .alpha./.beta.-fold contg. a seven-stranded .beta.-sheet flanked by seven helixes, a small domain contg. a four-stranded antiparallel .beta.-sheet flanked by three .alpha.-helixes, and an N-terminal segment contg. two .alpha.-helixes. The overall fold of the subunit is similar to those of the enzymes belonging to the fold-type I family represented by aspartate aminotransferase. However, CsdB has several structural features that are not obsd. in other families of the enzymes. A remarkable feature is that an .alpha.-helix in the lobe extending from the small domain to the large domain in one subunit of the dimer interacts with a .beta.-hairpin loop protruding from the large domain of the other subunit. The extended lobe and the protruded .beta.-hairpin loop form one side of a limb of each active site in the enzyme. The most striking structural feature of CsdB lies in the location of a putative catalytic residue; the side chain of Cys364 on the extended lobe of one subunit is close enough to interact with the .gamma.-atom of a modeled substrate in the active site of the subunit. Moreover, His55 from the other subunit is positioned so that it interacts with the .gamma.- or .beta.-atom of the substrate and may be involved in the catalytic reaction. This is the first report on three-dimensional structures of NifS homologs.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:466914 CAPLUS
DOCUMENT NUMBER: 131:254222
TITLE: A nifS-like gene, csdB, encodes an Escherichia coli counterpart of mammalian **selenocysteine** lyase. Gene cloning, purification, characterization and preliminary **x-ray** crystallographic studies
AUTHOR(S): Mihara, Hisaaki; Maeda, Masaki; Fujii, Tomomi; Kurihara, Tatsuo; Hata, Yasuo; Esaki, Nobuyoshi
CORPORATE SOURCE: Institute for Chemical Research, Kyoto University, Kyoto, 611-0011, Japan
SOURCE: Journal of Biological Chemistry (1999), 274(21), 14768-14772

CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB **Selenocysteine** lyase is a pyridoxal 5'-phosphate (PLP)-dependent enzyme that catalyzes the exclusive decompn. of L-**selenocysteine** to L-alanine and elemental selenium. An open reading frame, named csdB, from Escherichia coli encodes a putative protein that is similar to **selenocysteine** lyase of pig liver and cysteine desulfurase (NifS) of Azotobacter vinelandii. In this study, the csdB gene was cloned and expressed in E. coli cells. The gene product was a homodimer with the subunit Mr of 44,439, contained 1 mol of PLP as a cofactor per mol of subunit, and catalyzed the release of Se, SO2, and S from L-**selenocysteine**, L-cysteine sulfinic acid, and L-cysteine, resp., to yield L-alanine; the reactivity of the substrates decreased in this order. Although the enzyme was not specific for L-**selenocysteine**, the high specific activity for L-**selenocysteine** (5.5 units/mg compared with 0.019 units/mg for L-cysteine) supports the view that the enzyme can be regarded as an E. coli counterpart of mammalian **selenocysteine** lyase. The authors crystd. CsdB, the csdB gene product, by the hanging drop vapor diffusion method. The crystals were of suitable quality for **x-ray** crystallog. and belonged to the tetragonal space group P43212 with unit cell dimensions of a = b = 128.1 .ANG. and c = 137.0 .ANG.. Consideration of the Matthews parameter Vm (3.19 .ANG.3/Da) accounts for the presence of a single dimer in the crystallog. asym. unit. A native diffraction dataset up to 2.8 .ANG. resoln. was collected. This is the first crystallog. anal. of a protein of NifS/**selenocysteine** lyase family.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:380142 CAPLUS
DOCUMENT NUMBER: 131:155289
TITLE: The **crystal structure** of a reduced [NiFeSe] hydrogenase provides an image of the activated catalytic center
AUTHOR(S): Garcin, E.; Vernede, X.; Hatchikian, E. C.; Volbeda, A.; Frey, M.; Fontecilla-Camps, J. C.
CORPORATE SOURCE: Institut de Biologie Structurale JP Ebel, Laboratoire de Cristallographie et Cristallogenese des Proteines, CEA-CNRS, Grenoble, F-38027, Fr.
SOURCE: Structure (London) (1999), 7(5), 557-566
CODEN: STRUE6; ISSN: 0969-2126
PUBLISHER: Current Biology Publications
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [NiFeSe] hydrogenases are metalloenzymes that catalyze the reaction H2 .tautm. 2H+ + 2e-. They are generally heterodimeric, contain 3 Fe-S clusters in their small subunit and a Ni-Fe-contg. active site in their large subunit that includes a **selenocysteine** (SeCys) ligand. Here, the authors report the **x-ray crystal structure** at 2.15 .ANG. resoln. of periplasmic [NiFeSe] hydrogenase from Desulfomicrobium baculatum in its reduced, active form. A comparison of active sites of oxidized, as-prepd., Desulfovibrio gigas and the reduced D. baculatum hydrogenases showed that in the reduced enzyme the Ni-Fe distance was 0.4 .ANG. shorter than in the oxidized enzyme. In addn., the putative oxo ligand, detected in the as-prepd. D. gigas enzyme, was absent from the D. baculatum hydrogenase. The authors also obsd. higher-than-av. temp. factors for both the active site Ni-**selenocysteine** ligand and the neighboring Glu-18 residue, suggesting that both these moieties are involved in proton transfer between the active site and the mol. surface. Other differences between [NiFeSe] and [NiFe] hydrogenases were the presence of a 3rd [4Fe4S] cluster replacing the [3Fe4S] cluster found in the D. gigas enzyme, and a putative Fe center that substitutes the Mg2+ ion that has already been described at the C-terminus of the large subunit of 2 [NiFe] hydrogenases. The heterolytic cleavage of H2 seems to be mediated by the Ni center and the **selenocysteine** residue. In addn. to modifying the catalytic properties of the enzyme, the Se ligand might protect the Ni atom from

oxidn. It was concluded that the putative oxo ligand is a signature of inactive "unready" [NiFe] hydrogenases.

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:283901 CAPLUS
DOCUMENT NUMBER: 131:84505
TITLE: Crystallization and **X-ray** diffraction data of a tRNASec acceptor-stem helix
AUTHOR(S): Forster, Charlotte; Eickmann, Andrea; Schubert, Uwe; Hollmann, Susanne; Muller, Uwe; Heinemann, Udo; Furste, Jens Peter
CORPORATE SOURCE: Freie Universitat Berlin, Institut fur Biochemie, Berlin, 14195, Germany
SOURCE: Acta Crystallographica, Section D: Biological Crystallography (1999), D55(3), 664-666
CODEN: ABCRE6; ISSN: 0907-4449
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB TRNASec is a UGA suppressor tRNA which co-translationally inserts **selenocysteine** into proteins. Its eight-base-pair tRNASec acceptor stem, which contains key recognition elements, was synthesized using solid-phase phosphoramidite RNA chem. High-resoln. **X-ray** diffraction data were collected using synchrotron radiation under cryogenic cooling conditions. The crystals diffract to a maximal resoln. of 1.8 .ANG.. **X-ray** diffraction data were processed to 2.4 .ANG.. TRNASec microhelix crystallizes in space group R32, with cell consts. a = 47.02, b = 47.02, c = 373.03 .ANG., .alpha. = .beta. = 90, .gamma. = 120.degree.. The crystals contain three RNA mols. per asym. unit.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:766918 CAPLUS
DOCUMENT NUMBER: 130:121342
TITLE: Substituting **selenocysteine** for active site cysteine 149 of phosphorylating glyceraldehyde 3-phosphate dehydrogenase reveals a peroxidase activity
AUTHOR(S): Boschi-Muller, Sandrine; Muller, Sabine; Van Dorsselaer, Alain; Bock, August; Branlant, Guy
CORPORATE SOURCE: Faculte des Sciences, UMR 7567 CNRS-UHP, Maturation des ARN et Enzymologie Moleculaire, Vandoeuvre-Les-Nancy, 54506, Fr.
SOURCE: FEBS Letters (1998), 439(3), 241-245
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Replacing the essential Cys-149 by a **selenocysteine** in the active site of phosphorylating glyceraldehyde 3-phosphate dehydrogenase (GAPDH) from Bacillus stearothermophilus leads to a selenoGAPDH that mimics a selenoperoxidase activity. Satn. kinetics were obsd. with cumenyl and tert-Bu hydroperoxides, with a better catalytic efficiency for the arom. compd. The enzymic mechanism fits a sequential model where the formation of a ternary complex between the holoselenoenzyme, the 3-carboxy 4-nitrobenzenethiol used as the reductant and the hydroperoxide precedes product release. The fact that the selenoGAPDH is NAD-satd. supports a binding of hydroperoxide and reductant in the substrate binding site. The catalytic efficiency is similar to selenosubtilisins but remains low compared to selenoglutathione peroxidase. This is discussed in relation to what is known from the **X-ray crystal structures** of selenoglutathione peroxidase and GAPDHs.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:89364 CAPLUS

DOCUMENT NUMBER: 124:139771
TITLE: **Crystal structure** and mutants of interleukin-1 beta converting enzyme
INVENTOR(S): Wilson, Keith P.; Griffith, James P.; Kim, Eunice E.; Livingston, David J.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9535367	A1	19951228	WO 1995-US7619	19950616
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5856116	A	19990105	US 1995-450130	19950525
US 6057119	A	20000502	US 1995-450362	19950525
CA 2192485	AA	19951228	CA 1995-2192485	19950616
AU 9527055	A1	19960115	AU 1995-27055	19950616
AU 701759	B2	19990204		
EP 765388	A1	19970402	EP 1995-922329	19950616
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10504447	T2	19980506	JP 1995-502480	19950616
EP 1365020	A1	20031126	EP 2003-10692	19950616
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
AU 9896113	A1	19990304	AU 1998-96113	19981208
AU 733479	B2	20010517		

PRIORITY APPLN. INFO.:

US 1994-261582	A	19940617
AU 1995-27055	A3	19950616
WO 1995-US7619	W	19950616
EP 1995-922329	A3	19951228

AB Interleukin-1.beta. converting enzyme ("ICE") processes an inactive precursor to the pro-inflammatory cytokine, interleukin-1.beta.. The high-resoln. structure of human ICE crystd. in complex with an inhibitor is detd. by **X-ray** diffraction. The active site spans both the 10 and 20 kilodalton subunits. The accessory binding site is composed of residues from the p10 to p20 subunits that are adjacent to the two-fold axis of the crystal. The structure coordinates of the enzyme may be used to design novel classes of ICE inhibitors.

=> s selenomethionine and (crystal structure or three dimenssional structure) and x-ray
L2 120 SELENOMETHIONINE AND (CRYSTAL STRUCTURE OR THREE DIMENSSIONAL STRUCTURE) AND X-RAY

=> d 100-120 ibib abs

L2 ANSWER 100 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:518908 CAPLUS
DOCUMENT NUMBER: 129:227196
TITLE: Subcloning, crystallization and preliminary **x-ray** analysis of the signal receiver domain of ETR1, an ethylene receptor from Arabidopsis thaliana
AUTHOR(S): Grantz, Alexander A.; Muller-Dieckmann, Hans-Joachim; Kim, Sung-Hou
CORPORATE SOURCE: Structural Biology Division of Lawrence Berkeley National Laboratory and Department of Chemistry, University of California, Berkeley, CA, 95720, USA
SOURCE: Acta Crystallographica, Section D: Biological Crystallography (1998), D54(4), 690-692
CODEN: ABCRE6; ISSN: 0907-4449
PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The signal receiver domain of ETR1, an ethylene receptor from Arabidopsis thaliana, was subcloned and expressed in Escherichia coli and purified by affinity chromatog. Crystals of both native and a **selenomethionine**-substituted form of the receiver domain were obtained. Native crystals grew in 1.6M Li2SO4 and 0.1M HEPES pH 7.5 and once flash-frozen diffract to 2.1 .ANG. resoln. They belong to space group P41212 with unit-cell dimensions a = b = 48.4, c = 112.3 .ANG..
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 101 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:531351 CAPLUS
DOCUMENT NUMBER: 127:146474
TITLE: Expression, purification, characterization, and **x-ray** analysis of **selenomethionine** 215 variant of leukocyte collagenase
AUTHOR(S): Pieper, Michael; Betz, Michael; Budisa, Nediljko; Gomis-Rueth, Franz-Xaver; Bode, Wolfram; Tschesche, Harald
CORPORATE SOURCE: Fakultat fur Chemie und Biochemie, Universitat Bielefeld, Bielefeld, D-33615, Germany
SOURCE: Journal of Protein Chemistry (1997), 16(6), 637-650
CODEN: JPCHD2; ISSN: 0277-8033
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Matrix metalloproteinases belong to the superfamily of metzincins contg., besides a similar topol. and a strictly conserved zinc environment, a 1,4-tight turn with a strictly conserved Met residue at position 3 (the so called Met-turn). The distal S-CH3 moiety of this Met residue forms the hydrophobic basement of the 3 His residues liganding the catalytic Zn2+. To assess the importance of this Met residue, the authors expressed the recombinant catalytic domain of neutrophil collagenase (rHNC, residues Met-80-Gly-242) in the methionine auxotrophic Escherichia coli strain B834[DE3](hsd metB), with the 2 Met residues replaced by **selenomethionine** (SeMet). Complete replacement was confirmed by amino acid anal. and electrospray mass spectrometry. The folded and purified enzyme retained its catalytic activity, but showed modifications which were reflected in changed kinetic parameters. The Met-215 .fwdarw. SeMet substitution caused a decrease in conformational stability upon urea denaturation. The **x-ray crystal structure** of this SeMet-rHNC was virtually identical to that of the wild-type catalytic domain except for a very faint local disturbance around the S-Se substitution site.

L2 ANSWER 102 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:455118 CAPLUS
DOCUMENT NUMBER: 127:92156
TITLE: Crystallization of the RNA guanylyltransferase of Chlorella virus PBCV-1
AUTHOR(S): Doherty, Aidan J.; Hakansson, Kjell; Ho, C. Kiong; Shuman, Stewart; Wigley, Dale B.
CORPORATE SOURCE: Laboratory of Molecular Biophysics, University of Oxford, Oxford, OX1 3QU, UK
SOURCE: Acta Crystallographica, Section D: Biological Crystallography (1997), D53(4), 482-484
CODEN: ABCRE6; ISSN: 0907-4449
PUBLISHER: Munksgaard
DOCUMENT TYPE: Journal
LANGUAGE: English
AB MRNA guanylyltransferase, or capping enzyme (EC 2.7.7.50) (I) catalyzes the transfer of GMP from GTP to diphosphate-terminated RNA to form the cap structure, GpppN. Recombinant Chlorella virus I expressed in E. coli was purified, treated with GTP, and crystd. **X-ray** diffraction data were collected from these crystals as well as for a Hg deriv. obtained by soaking the crystals in thimerosal. **Selenomethionine**-I was purified and crystd. in a similar fashion. The space group was C2221 and the cell parameters were a = 93.3, b =

214.9, and c = 105.8 .ANG.. Two Hg atoms and 2 subsets of Se atoms were localized using difference Patterson and Fourier methods, suggesting that there are 2 mols. per asym. unit.

L2 ANSWER 103 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:293241 CAPLUS
DOCUMENT NUMBER: 127:2619
TITLE: Preparation of selenomethionyl proteins for phase determination
AUTHOR(S): Doublie, Sylvie
CORPORATE SOURCE: Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Methods in Enzymology (1997), 276(Macromolecular Crystallography, Part A), 523-530
CODEN: MENZAU; ISSN: 0076-6879
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The use of selenomethionyl proteins for phase detn. is growing in popularity for isomorphous replacement or multiwavelength anomalous dispersion expts. The procedures for engineering and crystg. selenomethionyl proteins are fairly straightforward and can be divided into 4 steps: expression, cell growth, purifn., and crystn. Each of these stages is described, and questions assocd. with storage and properties of selenomethionyl protein crystals are discussed.
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 104 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:188158 CAPLUS
DOCUMENT NUMBER: 126:289566
TITLE: Expression, crystallization, and preliminary **X-ray** analysis of a sialic acid-binding fragment of sialoadhesin in the presence and absence of ligand
AUTHOR(S): May, A. P.; Robinson, R. C.; Aplin, R. T.; Bradfield, P.; Crocker, P. R.; Jones, E. Y.
CORPORATE SOURCE: Lab. Molecular Biophysics, Univ. Oxford, Oxford, UK
SOURCE: Protein Science (1997), 6(3), 717-721
CODEN: PRCIEI; ISSN: 0961-8368
PUBLISHER: Cambridge University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Sialoadhesin is a macrophage-restricted cell surface receptor, consisting of 17 Ig domains, which mediates cell adhesion via the recognition of specific sialylated glycoconjugates. A functional fragment of sialoadhesin, comprising the N-terminal Ig domain, has been expressed in Chinese hamster ovary cells as both native (SnD1) and selenomethionyl (Se-SnD1) stop protein. The successful prodn. of 86% **selenomethionine**-incorporated protein represents a rare example of prodn. of selenium-labeled protein in mammalian cells. SnD1 and Se-SnD1 have been crystd. in the absence of ligand, and SnD1 has also been crystd. in the presence of its ligand 2,3-sialyllactose. The ligand-free crystals of SnD1 and Se-SnD1 were isomorphous, of space group P3121 or P3221, with unit cell dimensions a = b = 38.9 .ANG., c = 152.6 .ANG., .alpha. = .beta. = 90.degree., .gamma. = 120.degree., and diffracted to a max. resoln. of 2.6 .ANG.. Co-crystals contg. 2,3-sialyllactose diffracted to 1.85 .ANG. at a synchrotron source and belong to space group P212121, with unit cell dimensions a = 40.9 .ANG., b = 97.6 .ANG., c = 101.6 .ANG., .alpha. = .beta. = .gamma. = 90.degree..
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 105 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:734499 CAPLUS
DOCUMENT NUMBER: 126:86644
TITLE: A minimalist's approach to the phase problem - phasing selenomethionyl protein structures using Cu K.alpha. data
AUTHOR(S): Jaskolski, Mariusz; Wlodawer, Alexander

CORPORATE SOURCE: Macromolecular Structure Lab., NCI-Frederick Cancer Res. Dev. Center, Frederick, MD, 21702, USA
SOURCE: Acta Crystallographica, Section D: Biological Crystallography (1996), D52(6), 1075-1081
CODEN: ABCRE6; ISSN: 0907-4449
PUBLISHER: Munksgaard
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The feasibility of phasing protein structures through the use of the isomorphous and anomalous signal of selenomethionyl (Se-Met) deriv. and diffraction data collected with a std. lab. Cu K.alpha. **x-ray** source was investigated. Interpretable electron-d. maps were obtained for the core domain of avian sarcoma virus integrase, a typical medium-sized protein having 4 Met residues in a sequence of 156 amino acids. The r.m.s. difference between 3.1 .ANG. exptl. phases obtained from Se-Met Cu K.alpha. data and the final phases calcd. from the refined model is 55.degree.. A procedure combining single isomorphous replacement/single anomalous scattering phasing and solvent flattening for data based on a single Se-Met deriv. and Cu K.alpha. radiation was tested on this and another protein. The results are encouraging enough to indicate that such procedures might be recommended when a synchrotron source is not readily available.

L2 ANSWER 106 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:308695 CAPLUS
DOCUMENT NUMBER: 124:336581
TITLE: Crystallization and preliminary **X-ray** crystallographic studies of Escherichia coli xanthine phosphoribosyltransferase
AUTHOR(S): Vos, Siska; De Jersey, John; Martin, Jennifer L.
CORPORATE SOURCE: Centre Protein Structure, Function and Engineering, University Queensland, Australia
SOURCE: Journal of Structural Biology (1996), 116(2), 330-334
CODEN: JSBIEM; ISSN: 1047-8477
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Xanthine phosphoribosyltransferase (XPRT; EC 2.4.2.22) from Escherichia coli is a purine salvage enzyme which synthesizes the nucleotides GMP, XMP, and IMP. A mutant C59A, which is more stable than wild-type XPRT while retaining high activity, has been prepd. and crystd. to give three different crystal forms (A, B, and C). Form A crystals are orthorhombic (P21212), with unit cell dimensions a = 59.2 .ANG., b = 92.9 .ANG., c = 53.2 .ANG.. Form B crystals are monoclinic (C2) with unit cell dimensions a = 84.4 .ANG., b = 70.8 .ANG., c = 54.1 .ANG., and .beta. = 113.4.degree., and form C crystals are tetragonal (P41212 or P43212) with unit cell dimensions a,b = 94 .ANG., c = 167.5 .ANG.. Wild-type XPRT and a **selenomethionine** deriv. of C59A XPRT have also been crystd. in the orthorhombic form. The **selenomethionine** deriv. was prepd. by expressing XPRT in the usual E. coli strain without the need for a methionine auxotroph. Cells were grown in a methionine-deficient medium supplemented with **selenomethionine** which gave >95% incorporation. Both the wild-type and **selenomethionine** C59A XPRT crystals are isomorphous with C59A form A crystals.

L2 ANSWER 107 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:249034 CAPLUS
DOCUMENT NUMBER: 124:283104
TITLE: **Crystal Structure** of the Rat Liver Fructose-2,6-bisphosphatase Based on **Selenomethionine** Multiwavelength Anomalous Dispersion Phases
AUTHOR(S): Lee, Yong-Hwan; Ogata, Craig; Pflugrath, James W.; Levitt, David G.; Sarma, Ragupathy; Banaszak, Leonard J.; Pilkis, Simon J.
CORPORATE SOURCE: Departments of Biochemistry and Physiology, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Biochemistry (1996), 35(19), 6010-19
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The **crystal structure** of the recombinant fructose-2,6-bisphosphatase (Fru-2,6-P2ase) domain, which covers the residues between 251 and 440 of the rat liver bifunctional enzyme, 6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase, was detd. by multiwavelength anomalous dispersion phasing and refined at 2.5 .ANG. resoln. The **selenomethionine**-substituted protein was induced in the methionine auxotroph, Escherichia coli DL41DE3, purified, and crystd. in a manner similar to that of the native protein. Phase information was calcd. using the multiwavelength anomalous dispersion data collected at the **X-ray** wavelengths near the absorption edge of the K-shell .alpha. electrons of selenium. The Fru-2,6-P2ase domain has a core .alpha./.beta. structure, which consists of six stacked .beta.-strands, four parallel and two antiparallel. The core .beta.-sheet is surrounded by nine .alpha.-helixes. The catalytic site, as defined by a bound phosphate ion, is positioned near the C-terminal end of the .beta.-sheet and is close to the N-terminal end of an .alpha.-helix. The active site pocket is funnel-shaped. The narrow opening of the funnel is wide enough for a water mol. to pass. The key catalytic residues, including His7, His141, and Glu76, are near each other at the active site and probably function as general acids and/or bases during a catalytic cycle. The inorg. phosphate mol. is bound to an anion trap formed by Arg6, His7, Arg56, and His141. The core structure of the Fru-2,6-P2ase is similar to that of the yeast phosphoglycerate mutase and the rat prostatic acid phosphatase. However, the structure of one of the loops near the active site is completely different from the other family members, perhaps reflecting functional differences and the nanomolar range affinity of Fru-2,6-P2ase for its substrate. The imidazole rings of the two key catalytic residues, His7 and His141, are not parallel as in the yeast phosphoglycerate mutase. The **crystal structure** is used to interpret the existing chem. data already available for the bisphosphatase domain. In addn., the **crystal structure** is compared with two other proteins that belong to the histidine phosphatase family.

L2 ANSWER 108 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:202717 CAPLUS
DOCUMENT NUMBER: 124:253419
TITLE: **Crystal structure** analysis using a selenomethionyl protein
AUTHOR(S): Senda, Toshiya
CORPORATE SOURCE: Dep. Bio-Eng., Nagaoka Univ. Technol., Nagaoka, 940-21, Japan
SOURCE: Nippon Kessho Gakkaishi (1996), 38(1), 14-19
CODEN: NKEGAF; ISSN: 0369-4585
PUBLISHER: Nippon Kessho Gakkai
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Japanese

AB A review with 12 refs. on the use of selenomethionyl proteins in protein crystallog. is presented. **Selenomethionine** can be used as one of the heavy atom derivs. because of its sufficient phasing powder. In addn., the positions of selenium atoms can be easily detd. through the use of the difference Fourier technique. Using these positions as a guide, the amt. of labor needed for interpreting electron d. maps is much reduced. Here, we report on one example of structure detn. using a selenomethionyl protein as one of the heavy atom derivs. and give results of the anal. in relation to the use of selenomethionyl proteins in protein crystallog.

L2 ANSWER 109 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:140803 CAPLUS
DOCUMENT NUMBER: 124:168778
TITLE: Crystallization and preliminary **x-ray** characterization of the Methanothermus fervidus histones HMfA and HMfB
AUTHOR(S): Decanniere, Klaas; Sandman, Kathleen; Reeve, John N.; Heinemann, Udo
CORPORATE SOURCE: Forschungsgruppe Kristallographie, Max-Delbrueck-Centrum, Berlin, D-13122, Germany
SOURCE: Proteins: Structure, Function, and Genetics (1996), 24(2), 269-71

CODEN: PSFGEY; ISSN: 0887-3585
PUBLISHER: Wiley-Liss
DOCUMENT TYPE: Journal
LANGUAGE: English

AB HMfA and HMfB are histone proteins from the thermophilic archaeon, M. fervidus. They wrap DNA into nucleosome-like structures and appear to represent the basic core histone fold. Here, HMfA was crystd. in space groups P42212 and P212121. HMfB crystd. in space group P21212, whereas a **selenomethionine**-substituted variant, SeMet-HMfB, yielded crystals in C2221. In all crystal forms, HMfA, HMfB, or SeMet-HMfB may be present as homodimers.

L2 ANSWER 110 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:89364 CAPLUS
DOCUMENT NUMBER: 124:139771
TITLE: **Crystal structure** and mutants of interleukin-1 beta converting enzyme
INVENTOR(S): Wilson, Keith P.; Griffith, James P.; Kim, Eunice E.; Livingston, David J.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9535367	A1	19951228	WO 1995-US7619	19950616
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5856116	A	19990105	US 1995-450130	19950525
US 6057119	A	20000502	US 1995-450362	19950525
CA 2192485	AA	19951228	CA 1995-2192485	19950616
AU 9527055	A1	19960115	AU 1995-27055	19950616
AU 701759	B2	19990204		
EP 765388	A1	19970402	EP 1995-922329	19950616
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10504447	T2	19980506	JP 1995-502480	19950616
EP 1365020	A1	20031126	EP 2003-10692	19950616
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
AU 9896113	A1	19990304	AU 1998-96113	19981208
AU 733479	B2	20010517		

PRIORITY APPLN. INFO.: US 1994-261582 A 19940617
AU 1995-27055 A3 19950616
WO 1995-US7619 W 19950616
EP 1995-922329 A3 19951228

AB Interleukin-1.beta. converting enzyme ("ICE") processes an inactive precursor to the pro-inflammatory cytokine, interleukin-1.beta.. The high-resoln. structure of human ICE crystd. in complex with an inhibitor is detd. by **X-ray** diffraction. The active site spans both the 10 and 20 kilodalton subunits. The accessory binding site is composed of residues from the p10 to p20 subunits that are adjacent to the two-fold axis of the crystal. The structure coordinates of the enzyme may be used to design novel classes of ICE inhibitors.

L2 ANSWER 111 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:868941 CAPLUS
DOCUMENT NUMBER: 123:309191
TITLE: Expression, characterization and crystallographic analysis of telluromethionyl dihydrofolate reductase
AUTHOR(S): Boles, Jeffrey O.; Lewinski, Krzysztof; Kuncle, Marci G.; Hatada, Marcos; Lebioda, Lukasz; Dunlap, R. Bruce; Odom, Jerome D.
CORPORATE SOURCE: Dep. of Chemistry, Tennessee Tech. Univ., Cookeville,

TN, 38505, USA
SOURCE: Acta Crystallographica, Section D: Biological Crystallography (1995), D51(5), 731-9
CODEN: ABCRE6; ISSN: 0907-4449
PUBLISHER: Munksgaard
DOCUMENT TYPE: Journal
LANGUAGE: English
AB **Selenomethionine**-contg. proteins analyzed by multi-wavelength anomalous diffraction provide a facile means of addressing the phase problem, whose soln. is necessary to det. protein structures by **x-ray** crystallog. {Hendrickson (1991). Science, 254, 51-58}. Since this method requires synchrotron radiation, the authors sought to incorporate a true heavy atom into protein, allowing the soln. of the phase problem by more traditional methods of data collection. Media contg. TeMet alone or TeMet with low levels of Met failed to sustain growth of a methione auxotroph of Escherichia coli carrying the dihydrofolate reductase expression vector. Growth of the organism to stationary phase and incorporation of TeMet was obsd. when the culture was initiated in media contg. minimal Met levels and TeMet was added after induction with isopropyl-1-thio-.beta.-D-galactopyranoside. The purified enzyme exhibited properties similar to those of the native enzyme. At. absorption spectroscopy ad amino-acid anal. indicated that 40% of the methionines were replaced with TeMet. Sequence anal. did not indicate significant levels of replacement in the first three sites (1, 16 and 20), suggesting that TeMet was present only in the last two sites (42 and 92). Crystals of this enzyme were grown in the presence of methotrexate and were isomorphous with crystals of wild-type dihydrofolate reductase. Difference Fourier maps and restrained least-squares refinement showed no substitution at the first three methionines, while incorporation was seen at positions 42 and 92.

L2 ANSWER 112 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:788032 CAPLUS
DOCUMENT NUMBER: 123:192258
TITLE: Crystallization and preliminary **X-ray** diffraction studies of the human adenovirus serotype 2 proteinase with peptide cofactor
AUTHOR(S): Keefe, Lisa J.; Ginell, Stephan L.; Westbrook, Edwin M.; Anderson, Carl W.
CORPORATE SOURCE: Center Mechanistic Biology Biotechnology, Argonne National Laboratory, Argonne, IL, 60439, USA
SOURCE: Protein Science (1995), 4(8), 1658-60
CODEN: PRCIEI; ISSN: 0961-8368
PUBLISHER: Cambridge University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Recombinant human adenovirus serotype 2 proteinase (both native and **selenomethionine**-substituted) has been crystd. in the presence of the serotype 12, 11-residue peptide cofactor. The crystals (space group P3121 or P3221, one mol. per asym. unit, a = b = 41.3 .ANG., c = 197.0 .ANG.) grew in solns. contg. 20-40% 2-methyl-2,4-pentanediol (MPD), 0.1-0.2 M sodium citrate, and 0.1 M sodium HEPES, pH 5.0-7.5. Diffraction data (84% complete to 2.2 .ANG. resoln. with Rmerge of 0.0335) have been measured from cryo-preserved native enzyme crystals with the Argonne blue (1,024.times.1,024 pixel array) charge-coupled device detector at beamline X8C at the National Synchrotron Light Source (operated by Argonne National Lab.'s Structural Biol. Center). Addnl., diffraction data from **selenomethionine**-substituted proteinase, 65% complete to 2.0 .ANG. resoln. with Rmerge values ranging 0.05-0.07, have been collected at three **x-ray** energies at and near the selenium absorption edge. The authors have detd. three of the six selenium sites and are initiating a structure soln. by the method of multi-wavelength anomalous diffraction phasing.

L2 ANSWER 113 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:273503 CAPLUS
DOCUMENT NUMBER: 122:75021
TITLE: Crystallization and preliminary **x-ray** diffraction characterization of both a native and selenomethionyl VLA-4 binding fragment of VCAM-1

AUTHOR(S): Bottomley, M. J.; Robinson, R. C.; Driscoll, P. C.; Harlos, K.; Stuart, D. I.; Aplin, R. T.; Clements, J. M.; Jones, E. Y.; Dudgeon, T. J.
CORPORATE SOURCE: Dep. Biochemistry, Univ. Oxford, Oxford, OX1 3QU, UK
SOURCE: Journal of Molecular Biology (1994), 244(4), 464-8
CODEN: JMOBAK; ISSN: 0022-2836
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Sol. fragments of the extracellular region of vascular cell adhesion mol. 1 (VCAM-1) expressed in Escherichia coli retain functional adhesive activity. An integrin (VLA-4) binding fragment consisting of the N-terminal two Ig-like domains (VCAM-d1,2) has been crystd. The crystals belong to space group P212121 with cell dimensions of a = 52.7 .ANG., b = 66.5 .ANG., c = 113.2 .ANG. and contain two mols. in the crystallog. asym. unit. A batch of protein produced in the std. E. coli strain (HW1110), but grown in the presence of **selenomethionine** enriched media, showed 85% incorporation of selenium in place of sulfur at methionine residues. The selenomethionyl VCAM-d1,2 was crystd. by microseeding techniques initially using the native crystals for nucleation. Both native and selenomethionyl crystals diffract **X-rays** to a min. Bragg spacing of 1.8 .ANG..

L2 ANSWER 114 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:452529 CAPLUS
DOCUMENT NUMBER: 121:52529
TITLE: Structure of the gene V protein of bacteriophage f1 determined by multiwavelength **x-ray** diffraction on the selenomethionyl protein
AUTHOR(S): Skinner, Matthew M.; Zhang, Hong; Leschnitzer, Dale H.; Guan, Yue; Bellamy, Henry; Sweet, Robert M.; Gray, Carla W.; Konings, Ruud N. H.; Wang, Andrew H. J.; Terwilliger, Thomas C.
CORPORATE SOURCE: Life Sci. Div., Los Alamos Natl. Lab., Los Alamos, NM, 87545, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1994), 91(6), 2071-5
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The **crystal structure** of the dimeric gene V protein of bacteriophage f1 was detd. using multiwavelength anomalous diffraction on the **selenomethionine**-contg. wild-type and isoleucine-47 .fwdarw. methionine mutant proteins with **x-ray** diffraction data phased to 2.5 .ANG. resoln. The structure of the wild-type protein has been refined to an R factor of 19.2% using native data to 1.8 .ANG. resoln. The structure of the gene V protein was used to obtain a model for the protein portion of the gene V protein-single-stranded DNA complex.

L2 ANSWER 115 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:211768 CAPLUS
DOCUMENT NUMBER: 120:211768
TITLE: Production of recombinant selenomethionyl proteins in Escherichia coli can lead to direct phasing for three-dimensional structure determination by **x-ray** crystallography
AUTHOR(S): Horton, John Raymond
CORPORATE SOURCE: Columbia Univ., New York, NY, USA
SOURCE: (1992) 340 pp. Avail.: Univ. Microfilms Int., Order No. DA9313612
From: Diss. Abstr. Int. B 1993, 54(1), 121-2
DOCUMENT TYPE: Dissertation
LANGUAGE: English

AB Unavailable

L2 ANSWER 116 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:157920 CAPLUS
DOCUMENT NUMBER: 120:157920
TITLE: MAD phasing: Bayesian estimates of FA
AUTHOR(S): Terwilliger, Thomas C.
CORPORATE SOURCE: Life Sci. Div., Los Alamos Natl. Lab., Los Alamos, NM,

87545, USA
SOURCE: Acta Crystallographica, Section D: Biological Crystallography (1994), D50(1), 11-16
CODEN: ABCRE6; ISSN: 0907-4449
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A Bayesian approach is applied to the calcn. of Patterson functions and cross-Fourier maps in the anal. of multi-wavelength anomalous-diffraction (MAD) data. This procedure explicitly incorporates information available a priori on the likely magnitudes of partial structure factors (FA) corresponding to the anomalously scattering atoms, uses weighted-av. ests. of FA, and incorporates ests. of errors in the data that are not represented in the instrumental uncertainties. The method is demonstrated by application to MAD data collected on **selenomethionine**-contg. gene V protein.

L2 ANSWER 117 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:186489 CAPLUS
DOCUMENT NUMBER: 118:186489
TITLE: Purification, characterization, crystallization and **x-ray** analysis of **selenomethionine**-labeled hydroxymethylbilane synthase from Escherichia coli
AUTHOR(S): Haedener, Alfons; Matzinger, Peter K.; Malashkevich, Vladimir N.; Louie, Gordon V.; Wood, Stephen P.; Oliver, Philip; Alefounder, Peter R.; Pitt, Andrew R.; Abell, Chris; Battersby, Alan R.
CORPORATE SOURCE: Inst. Org. Chem., Univ. Basel, Basel, CH-4056, Switz.
SOURCE: European Journal of Biochemistry (1993), 211(3), 615-24
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Hydroxymethylbilane synthase (HMBS) catalyzes the conversion of porphobilinogen into hydroxymethylbilane, a linear tetrapyrrolic intermediate in the biosynthesis of hemes, chlorophylls, vitamin B12 and related macrocycles. A recently reported new strategy was employed to obtain **x-ray** phase information, i. e., the collection of multiwavelength anomalous diffraction data from a crystal of a seleno-L-methionine (SeMet)-labeled variant of the protein. Here, HMBS (38,268 Da) of E. coli, in which all (6) methionine (Met) residues were replaced by SeMet, was expressed and purified. Complete replacement, as shown by amino acid compn. anal. and by electrospray mass spectrometry, was achieved by growing the Met-requiring mutant E. coli PO1562 carrying the plasmid pPA410 in a medium contg. 50 mg/L SeMet as the sole source of Met. [SeMet]HMBS exhibited full enzyme activity, as reflected by unchanged steady-state kinetic parameters relative to native enzyme. Rhombohedral crystals of [SeMet]HMBS were grown at the pH optimum (7.4) of the enzyme (solns. contg. 30 mg/mL protein, 0.4 mM EDTA, 20 mM dithiothreitol, 3M NaCl and 15 mM Bistris-propane buffer were equilibrated by vapor diffusion at 20.degree. against reservoirs of satd. NaCl). However, being very thin plates, these crystals were not suitable for **x-ray** anal. Alternatively, rectangular crystals were obtained at pH 5.3 using conditions based on those reported for wild-type HMBS [sitting drops of 50 .mu.L contg. 6-7 mg/mL protein, 0.3 mM EDTA, 15 mM dithiothreitol, 10% (mass/vol.) poly(ethylene glycol) 6000 and 0.01% NaN3 in 0.1M NaOAC were equilibrated by vapor diffusion at 20.degree. against a reservoir of 10-20 mg solid dithiothreitol]. **X-ray** diffraction data of the crystals were complete to 93.8% at 0.21 nm resoln. and showed that [SeMet]HMBS and native HMBS crystd. isomorphously. A difference Fourier map using FSeMet - Fnative and phases derived from the native structure, which was recently detd. independently by multiple isomorphous replacement, showed pos. difference peaks centered at or close to where the S atoms of the Met side-chains appear in the native structure. In addn., paired pos./neg. peaks in the difference map near the cofactor of HMBS indicated conformational differences in the active site, probably due to differences in the state of oxidn. of the cofactor in the 2 cryst. samples.

L2 ANSWER 118 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:15350 CAPLUS

DOCUMENT NUMBER: 114:15350
TITLE: Effect of the anisotropy of anomalous scattering on the MAD phasing method
AUTHOR(S): Fanchon, Eric; Hendrickson, Wayne A.
CORPORATE SOURCE: Howard Hughes Med. Inst., Columbia Univ., New York, NY, 10032, USA
SOURCE: Acta Crystallographica, Section A: Foundations of Crystallography (1990), A46(10), 809-20
CODEN: ACACEQ; ISSN: 0108-7673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The anal. of **x-ray** diffraction intensities is complicated by the anisotropy of anomalous scattering (AAS) that can occur due to resonance assocd. with transitions between core electrons and valence MOs. Substantial AAS has been obsd. directly in diffraction data near the K edge of Se in selenolanthionine (Templeton and Templeton, (1988) and in pleiochroism of **x-ray** absorption in selenobiotinyl streptavidin (H. et al., 1989). The impact of AAs on the multiple-wavelength anomalous diffraction (MAD) method for phase detn. is of particular interest in the context of this chem. state of Se in the light of a general method that has been developed to incorporate **selenomethionine** into proteins for use in MAD phasing (H. et al., 1990). The first step of the MAD phasing method necessarily assumes that the anomalous-scattering factors are isotropic and the first aim is to evaluate the effect of this approxn. on initially detd. phases. To obtain ultimate phases free from the effects of anisotropy, a least-squares procedure was written in which global parameters (i.e. pertaining to the whole data set) are refined simultaneously with local parameters (e.g. pertaining to a given node h). The AAS is taken explicitly into account by considering f' and f'' as tensors instead of scalars (Templeton and Templeton, 1982), and the components of the f' and f'' tensors are among the refinable global parameters. The effectiveness of this procedure is tested with data simulated from the refined at. model of selenobiotinyl streptavidin. The application of this procedure to actual Photon Factory measurements is also described. AAS does not cripple the MAD method, and phases uncorrupted by these effects can be recovered.

L2 ANSWER 119 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1990:511594 CAPLUS
DOCUMENT NUMBER: 113:111594
TITLE: Expression, purification, and crystallization of natural and selenomethionyl recombinant ribonuclease H from Escherichia coli
AUTHOR(S): Yang, Wei; Hendrickson, Wayne A.; Kalman, Eva T.; Crouch, Robert J.
CORPORATE SOURCE: Dep. Biochem. Mol. Biophys., Columbia Univ., New York, NY, 10032, USA
SOURCE: Journal of Biological Chemistry (1990), 265(23), 13553-9
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English

AB RNase H from E. coli is an endonuclease that specifically degrades the RNAs of RNA:DNA hybrids. The enzyme is a single polypeptide chain of 155 amino acid residues, of which 4 are methionines. To solve the crystallog. three-dimensional structure of E. coli RNase H by the multiwavelength anomalous diffraction technique, methionine auxotrophic strains of E. coli were constructed that overexpress selenomethionyl RNase H. MIC88 yields about 10 mg of selenomethionyl RNase H per L of culture, which is comparable to the overexpression of the natural recombinant protein. Both proteins were purified to homogeneity and were crystd. isomorphously in the presence of sulfate. These are Type I crystals of space group P212121 with the cell parameters a = 41.8, b = 86.4, c = 36.4 .ANG., one monomer per asym. unit, and .apprx.36% (vol./vol.) solvent. Crystals of both proteins diffract to beyond 2-.ANG. Bragg spacings and are relatively durable in an **x-ray** beam. On replacement of sulfate with NaCl, crystals of natural RNase H grow as Type I' (very similar to Type I) at pH between 7.0 and 8.0; at pH 8.8, crystals of Type II are obtained in space group P212121 with a = 44.3, b - 87.3, and c = 35.7 .ANG.. Type II crystals can be converted to Type I by soaking in phosphate buffer.

L2 ANSWER 120 OF 120 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1990:420354 CAPLUS
DOCUMENT NUMBER: 113:20354
TITLE: Selenomethionyl proteins produced for analysis by multiwavelength anomalous diffraction (MAD): a vehicle for direct determination of three-dimensional structure
AUTHOR(S): Hendrickson, Wayne A.; Horton, John R.; LeMaster, David M.
CORPORATE SOURCE: Howard Hughes Med. Inst., Columbia Univ., New York, NY, 10032, USA
SOURCE: EMBO Journal (1990), 9(5), 1665-72
CODEN: EMJODG; ISSN: 0261-4189
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An expression system has been established for the incorporation of **selenomethionine** into recombinant proteins produced from plasmids in Escherichia coli. Replacement of methionine by **selenomethionine** is demonstrated at the level of 100% for both T4 and E. coli thioredoxins. The natural recombinant proteins and the selenomethionyl variants of both thioredoxins crystallize isomorphously. Anomalous scattering factors were deduced from synchrotron **x-ray** absorption measurements of crystals of the selenomethionyl proteins. Taken with ref. to experience in the structural anal. of selenobiotinyl streptavidin by the method of MAD, these data indicate that recombinant selenomethionyl proteins analyzed by MAD phasing offer a rather general means for the elucidation of at. structures.

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=> file .nash

=> s pneumoniae and acyl carrier protein synthase and (selenocysteine or selenomethionine)
L1 0 FILE MEDLINE
L2 2 FILE CAPLUS
L3 0 FILE SCISEARCH
L4 0 FILE LIFESCI
L5 0 FILE BIOSIS
L6 0 FILE EMBASE

TOTAL FOR ALL FILES
L7 2 PNEUMONIAE AND ACYL CARRIER PROTEIN SYNTHASE AND (SELENOCYSTEINE OR SELENOMETHIONINE)

=> d ibib abs

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:282044 CAPLUS
DOCUMENT NUMBER: 138:283319
TITLE: Purification, characterization and crystal structure of Streptococcus **pneumoniae acyl carrier protein synthase** for use in diagnostics, antibacterial drug design, and biosensors
INVENTOR(S): Chirgadze, Nicholas Yuri; Briggs, Stephen Lyle; Zhao, Genshi; McAllister, Kelly Ann
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 158 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003068802	A1	20030410	US 2001-897645	20010629

PRIORITY APPLN. INFO.: US 2000-215577P P 20000630
AB Provided are methods of purifying and crystg. Streptococcus

pneumoniae acyl carrier protein synthase (AcpS) enzyme, crystals of AcpS, the use of such crystals to det. the three-dimensional structure of AcpS enzymes, and the three-dimensional structure of AcpS. The three-dimensional crystal structure of AcpS can be used in medical diagnostics to produce antibodies that permit detection of Streptococcus **pneumoniae** both in vitro and in vivo. The three-dimensional crystal structure of AcpS can also be used in pharmaceutical discovery and development to identify and design compds. that inhibit the biochem. activity of AcpS enzyme in bacteria. Inhibitory compds. identified in this way can be optimized by structure/activity studies to develop antibacterial pharmaceutical compds. useful for the prevention or treatment of bacterial infections.

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L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:261864 CAPLUS
DOCUMENT NUMBER: 138:282444
TITLE: Cloning, purification and characterization of polypeptides from pathogenic bacteria involved in membrane biosynthesis, and drug screening and drug design applications
INVENTOR(S): Edwards, Aled; Dharamsi, Akil; Vedadi, Masoud; Alam, Muhammad Zahoor; Awrey, Donald; Beattie, Bryan; Canadien, Veronica; Domagala, Megan; Houston, Simon; Kanagarajah, Dhushy; Li, Qin; Mansoury, Kamran; McDonald, Merry-Lynn; Necakov, Sasha; Ng, Ivy; Pinder, Benjamin; Sheldrick, Bay; Vallee, Francois; Viola, Cristina; Wrezel, Olga
PATENT ASSIGNEE(S): Affinium Pharmaceuticals, Inc., Can.
SOURCE: PCT Int. Appl., 312 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003027139	A2	20030403	WO 2002-CA1443	20020924

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AB The present invention relates to polypeptide targets for pathogenic bacteria. A no. of antimicrobial target enzymes and proteins have been identified, expressed, and purified from Staphylococcus aureus, Helicobacter pylori, Streptococcus **pneumoniae**, and Pseudomonas aeruginosa. Cloning, the nucleotide sequences and the encoded amino acid sequences of genes ftsZ, fabZ, acpS, murD, murC, fabH, tagD, obg, and fabG from S. aureus, H. pylori, S. **pneumoniae**, and P. aeruginosa are disclosed. The invention also provides biochem. and biophys. characteristics of those polypeptides. The polypeptides are characterized by using mass spectrometry, NMR, x-ray crystallog., and bioinformatics anal. The polypeptides of the invention can be used for drug screening, drug design, in diagnostic assays and in pharmacol. applications.

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